Boiling Point (Range)

201-15046B

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E560

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the calculation method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured boiling point data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential boiling point range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific boiling point value. Actual boiling point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the boiling point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E560

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated BP (°C)	Measured* BP (°C)
Isoprene	34.95	34.0
n-pentane	46.01	36.0
1,3-cyclopentadiene	69.17	41.0
Isohexane	56.26	63.2
n-hexane	71.53	68.7
methylcyclopentane	80.34	71.8
benzene	102.24	80.0
toluene	125.72	110.6
m-xylene	148.29	139.1
styrene	146.65	145.0
dicyclopentadiene	176.78	170.0
naphthalene	231.64	217.9

* Experimental values from EPIWIN database.
The data represent a potential boiling point range for substances represented by the 19 CAS numbers under Test Substance.

Test Substance:

The High Benzene Naphthas Category includes the following CAS numbers:

64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy aromatic
67891-80-9	Distillates, petroleum, light aromatic
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E560

	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated boiling points for some representative constituents that are present in the category streams vary from 34.95 to 231.64°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 34.0 to 217.9°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the 19 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Boiling point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E560

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Boiling Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E568

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Light Source:	Not applicable
Light Spectrum: • **Wave length value (upper/lower)**	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Not applicable
Direct Photolysis:** • **Results: half-life, % degradation, quantum yield**	**Summary** In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the High Benzene Naphthas Category. The High Benzene Naphthas Category includes ten process streams: • **Pyrolysis Gasoline** • **Pyrolysis C6 Fraction** • **Pyrolysis C6-C8 Fraction** • **Pyrolysis C5-C6 Fraction** • **Hydrotreated C6 Fraction**

- **Hydrotreated C6-C7 Fraction**
- **Hydrotreated C6-C8 Fraction**
- **Quench Loop Pyrolysis Oil and Compressor Oil**
- **Recovered Oil from Waste Water Treatment**
- **Extract from Benzene Extraction**

Nineteen CAS numbers (see Test Substance) identify products derived from these process streams. As discussed below, the reaction process involved in direct photolysis occurs when sufficient light energy excites a molecule to the degree that a structural transformation occurs. In general, substances in this category do not contain component chemicals that will undergo direct photolysis.

The High Benzene Naphthas Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and co-processed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated High Benzene Naphthas.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the ten process streams in this category are:

- **Pyrolysis Gasoline** (Pygas) consists predominantly of C5+ hydrocarbons produced by the ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the debutanizer, (2) oils separated from furnace effluent quench systems, and (3) "drips" or condensate resulting from compression of the cracked gas. The oils from the quench systems and the "drips" may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be

transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present at a level greater than about 5%. The benzene concentration of Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams.

- **Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables.

    1. **Pyrolysis C5-C6 Fraction** has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.

    2. **Pyrolysis C6 Fraction** has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.

    3. **Pyrolysis C6-C8 Fraction** has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.

- **Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions)** are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for

	example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation. 1. **Hydrotreated C6 Fraction** is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of 75%. 2. **Hydrotreated C6-C7 Fraction** has a carbon number distribution that is predominantly C6-C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene. 3. **Hydrotreated C6-C8 Fraction** has a reported typical composition of 40 to 60% benzene, 10 to 25% toluene, and 3 to 10% C8 aromatics. • **Quench Loop Pyrolysis Oil and Compressor Oil** (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to 11% toluene. • **Recovered Oil from Wastewater Treatment** can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information has been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an isolated intermediate.

- **Extract from Benzene Extraction** are hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) which are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered. The carbon number distribution for this stream is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1% xylenes.

Photolysis of Hydrocarbons

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (2). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (2). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (2). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima (λ_{max}) and associated molar absorptivities (ε) for selected unsaturated hydrocarbons are shown below (2):

	l below 290 nm		**l above 290 nm**	
Hydrocarbon	λ_{max}	ε	λ_{max}	ε
Ethylene	193	10,000	-	-
Benzene	255	215	-	-
Styrene	244	12,000	-	-
	282	450		
Naphthalene	221	100,000	311	250
	270	5,000		

	Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the High Benzene Naphthas category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2). Products in the High Benzene Naphthas Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA. 2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA. 3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.
Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	Not applicable
Degradation Products:** • **Note: Identification, concentration**	Unknown

Photodegradation (Direct)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E568

Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha
Conclusion:	Not applicable
Reliability:	These data represent a key study for characterizing the potential of substances in the High Benzene Naphthas Category to undergo direct photodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2003. Photodegradation (Direct): High Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Direct). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E567

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling

	68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	**Summary** In the environment, hydrolysis will not contribute to the degradation of chemicals in the High Benzene Naphthas Category. The High Benzene Naphthas Category includes ten process streams: • **Pyrolysis Gasoline** • **Pyrolysis C6 Fraction** • **Pyrolysis C6-C8 Fraction** • **Pyrolysis C5-C6 Fraction** • **Hydrotreated C6 Fraction** • **Hydrotreated C6-C7 Fraction** • **Hydrotreated C6-C8 Fraction** • **Quench Loop Pyrolysis Oil and Compressor Oil** • **Recovered Oil from Waste Water Treatment** • **Extract from Benzene Extraction**

Nineteen CAS numbers (see Test Substance) identify substances derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur.

The High Benzene Naphthas Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. In some cases, petroleum refinery streams may be combined with intermediate streams from the ethylene unit and co-processed to produce these products. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C11, through components boiling at 650°F or higher. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated High Benzene Naphthas.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the ten process streams in this category are:

- **Pyrolysis Gasoline** (Pygas) consists predominantly of C5+ hydrocarbons produced by the ethylene cracking furnaces. Typically the stream is derived from (1) the bottoms product from the debutanizer, (2) oils separated from furnace effluent quench systems, and (3) “drips” or condensate resulting from compression of the cracked gas. The oils from the quench systems and the “drips” may be stabilized to remove lights before blending with Pygas from the other sources. Depending on the plant configuration, Pygas may contain all of these intermediate streams, or the quench oils and stabilized drips may be transferred as separate streams. Low concentrations (e.g. 3% total) of C4 and lighter hydrocarbons may be present in the stream. A detailed analysis of Pygas may identify 60 or more hydrocarbon components or component groups, primarily unsaturated hydrocarbons and aromatics. Benzene, toluene, and dicyclopentadiene together may account for more than 50% of a Pygas stream and typically no other single component is present

at a level greater than about 5%. The benzene concentration of Pygas is typically about 40% and the reported values range from 15 to 62%. The concentrations of individual hydrocarbon components in Pygas vary depending on the type of feedstock used by the ethylene plant, the mode of operation of the cracking furnaces (i.e. severity) and the ethylene process configuration. One non-typical Pygas stream is reported to contain vinylacetate at a concentration of up to about 10%. Vinylacetate is not typically found in ethylene process streams.

- **Pyrolysis Gasoline Fractions (C5-C6, C6, and C6-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this separation. Similar to the situation for Pygas, the composition of these fractions vary depending on the ethylene process feedstock and the other operating variables.

  1. **Pyrolysis C5-C6 Fraction** has a carbon number distribution that is predominantly C5 to C6. One typical composition for this stream is reported as 70% benzene and 10% pentenes.

  2. **Pyrolysis C6 Fraction** has a carbon number distribution that is predominantly C6. Reported compositions vary from 35 to 77% benzene, 0.5 to 5% toluene with the balance primarily C6 non-aromatics, which are expected to be largely unsaturates.

  3. **Pyrolysis C6-C8 Fraction** has a carbon number distribution that is predominantly C6 to C8. The reported compositions range from 30 to 80% benzene, 15 to 25% toluene and 3 to 23% C8 aromatics.

- **Hydrotreated Pyrolysis Fractions (C6, C6-C7, and C6-C8 Fractions)** are Pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst to saturate or partially saturate diolefins and/or olefins. In some cases, petroleum refinery streams such as a C6 reformate fraction are combined with the pyrolysis gasoline prior to this step. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained olefins to saturated hydrocarbons. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (benzene, toluene, or xylenes) is subjected to two-stage hydrogenation. Pygas fractions may be

forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Hydrotreated Pyrolysis fractions may be the result of either one- or two-stage hydrogenation.

1. **Hydrotreated C6 Fraction** is very similar to the Pyrolysis C6 fraction except that the non-aromatics present in the hydrotreated stream are essentially all saturates. The reported composition for the Hydrotreated C6 stream indicates typical benzene content of 75%.

2. **Hydrotreated C6-C7 Fraction** has a carbon number distribution that is predominantly C6-C7 and the reported values indicate 40 to 70% benzene, and 3 to 15% toluene.

3. **Hydrotreated C6-C8 Fraction** has a reported typical composition of 40 to 60% benzene, 10 to 25% toluene, and 3 to 10% C8 aromatics.

- **Quench Loop Pyrolysis Oil and Compressor Oil** (Pyoil) represents higher boiling hydrocarbons that condense in the water quench system of an ethylene plant, typically at an ethylene unit cracking ethane, propane or butane. The stream can also include liquids collected at the cracked gas compressor knock out drums, which may include compressor injection oil. The carbon number distribution for Pyoil is C4 (or even lower) through heavier hydrocarbons such as naphthalene or even heavier. The reported typical composition includes 10 to 22% benzene and 5 to 11% toluene.

- **Recovered Oil from Wastewater Treatment** can be expected to be of variable composition and made up largely of the components found in Pygas. No composition data or process specific information has been reported. Typically, water streams at ethylene units are processed to separate hydrocarbons from the water so that the water can be reused to generate steam for process-contact use (dilution steam for the cracking furnaces) or so that excess water can be forwarded to treatment prior to discharge or reuse. Water processing typically includes mechanical and gravity separation and steam or gas stripping. Hydrocarbons separated from the water in these systems are not usually isolated from the process. However, at least in one case, the Recovered Oil from Wastewater Treatment has been reported as an isolated intermediate.

- **Extract from Benzene Extraction** are hydrotreated pyrolysis fractions containing aromatics (most commonly benzene or benzene and toluene) which are typically charged to extraction or extractive distillation units where the mixed aromatics are recovered. The carbon number distribution for this stream is predominantly C6 to C8. A reported typical concentration indicates 60 to 75% benzene, 25 to 40% toluene and 0 to 1%

xylenes.

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (2,3). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (3) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the High Benzene Naphthas Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4).

The substances in the High Benzene Naphthas Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the High Benzene Naphthas Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

References

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.
3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.
4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E567

	Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	These data represent a key study for characterizing the potential of substances in the High Benzene Naphthas Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2003. Hydrolysis High Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Hydrolysis. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E^6 OH radicals/cm^3
Direct Photolysis:** **Results: half-life, % degradation, quantum yield**	Not applicable

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	**The High Benzene Naphthas Category** High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated High Benzene Naphthas. The 12 chemicals selected to represent the atmospheric oxidation potential of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge. **Atmospheric Oxidation of Hydrocarbons** In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH-radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993). AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals. Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

Indirect Photolysis: (cont'd)**

Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life

Chemical	Calculated* half-life (hrs)	OH- Rate Constant (cm^3/molecule-sec)
Isoprene	1.2	105.1 E^{-12}
n-pentane	31.7	4.0 E^{-12}
1,3-cyclopentadiene	0.9	142.6 E^{-12}
Isohexane	22.4	5.7 E^{-12}
n-hexane	23.5	5.5 E^{-12}
methylcyclopentane	22.7	5.7 E^{-12}
benzene	65.8	1.9 E^{-12}
toluene	24.6	5.2 E^{-12}
m-xylene	9.5	13.6 E^{-12}
styrene	4.6	28.1 E^{-12}
dicyclopentadiene	1.1	119.2 E^{-12}
naphthalene	5.9	21.6 E^{-12}

* Atmospheric half-life values are based on a 12-hr day.

More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001).

References:

1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem*. **7**:435-442.

2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.

3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299.

4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

Degradation Products:**

- **Note: Identification, concentration**

Unknown

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha
Conclusion:	Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 0.9 to 65.8 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E570

Reference:	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 10/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Indirect). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

** In IUCLID, provide additional discussion if needed in the results freetext

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E563

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. *J. Pharm. Sci*. 84:83-92.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured log K_{ow} data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential log K_{ow} range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific log K_{ow} value. Actual log K_{ow} ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the log K_{ow} range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E563

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated log K_{ow} @ 25°C	Measured* log K_{ow} @ 25°C
Isoprene	2.58	2.42
n-pentane	2.80	3.39
1,3-cyclopentadiene	2.25	na
Isohexane	3.21	3.60
n-hexane	3.29	3.90
methylcyclopentane	3.10	3.37
benzene	1.99	2.13
toluene	2.54	2.73
m-xylene	3.09	3.20
styrene	2.89	2.95
dicyclopentadiene	3.16	na
naphthalene	3.17	3.30

* Experimental values from EPIWIN database.
na = not available
The data represent a potential log K_{ow} range for substances represented by the 19 CAS numbers under Test Substance.

Test Substance:

The High Benzene Naphthas Category includes the following CAS numbers:

64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy aromatic
67891-80-9	Distillates, petroleum, light aromatic
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated log K_{ow} for some representative constituents that are present in the category streams vary from 1.99 to 3.29 @ 25°C. The measured log K_{ow} of these same constituents vary from 2.13 to 3.90 @ 25°C. Although this does not define the actual log K_{ow} of the category streams, it offers an indication of a range that might be expected to encompass the log K_{ow} of these complex streams with variable compositions. Log K_{ow} values outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential log K_{ow} range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log K_{ow} range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Log K_{ow} values were calculated by the KOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E563

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Partition Coefficient. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E561

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. The Gold and Ogle Method is described by Lyman, W.J., 1985, In: Environmental Exposure from Chemicals. Volume 1. Neely, W.B. and Blau, G.E. (eds), Boca Raton, FL, CRC Press, Inc., Chapter 2.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured melting point data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential melting point range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific melting point value. Actual melting point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the melting point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Substance Constituent	Calculated MP (°C)	Measured* MP (°C)
Isoprene	-118.89	-145.9
n-pentane	-106.92	-129.7
1,3-cyclopentadiene	-91.83	-85.0
Isohexane	-105.80	-162.9
n-hexane	-93.84	-95.3
methylcyclopentane	-85.82	-142.5
benzene	-77.92	5.5
toluene	-59.17	-94.9
m-xylene	-40.69	-47.8
styrene	-48.31	-31.0
dicyclopentadiene	-16.78	32.0
naphthalene	5.01	80.2

* Experimental values from EPIWIN database.
The data represent a potential melting point range for substances represented by the 19 CAS numbers under Test Substance.

Test Substance:

The High Benzene Naphthas Category includes the following CAS numbers:

64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy aromatic
67891-80-9	Distillates, petroleum, light aromatic
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E561

Test Substance: (continued)	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated melting points for some representative constituents that are present in the category streams vary from -118.89 to 5.01 °C. The measured melting points of these same constituents vary from -162.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the 19 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Melting point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Melting Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E569

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program (1). Measured input values were also used where available and obtained from the EPIWIN database (1). Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E569

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

Calculated partitioning data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential distribution for substances represented by the 19 CAS numbers under Test Substance. Actual distribution of substances in this category will vary dependent on their constituent composition.

Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the boiling point range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

The range of distribution data for constituent chemicals in each of the compartments can be used as an estimate of the partitioning behavior for category substances.

The following Mackay Level I model distribution values for representative constituents of substances in this category were determined using physicochemical input data calculated using the EPIWIN program:

	Calculated* Percent Distribution			
Chemical	Air	Water	Soil	Sediment
Isoprene	99.97	0.02	0.01	-
n-pentane	99.97	0.02	0.01	-
1,3-cyclopentadiene	99.93	0.06	0.01	-
Isohexane	99.96	0.02	0.02	-
n-hexane	99.95	0.02	0.02	-
methylcyclopentane	99.94	0.03	0.03	-
benzene	98.46	1.42	0.12	-
toluene	98.17	1.40	0.43	-
m-xylene	97.19	1.33	1.45	0.03
styrene	95.55	2.61	1.80	0.04
dicyclopentadiene	98.00	0.87	1.11	0.02
naphthalene	24.47	32.28	42.28	0.94

* Distribution values determined using calculated input data from EPIWIN program

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E569

Results: (cont'd)

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

	Measured** Percent Distribution			
Chemical	Air	Water	Soil	Sediment
Isoprene	99.96	0.03	0.01	-
n-pentane	99.99	0.01	-	-
1,3-cyclopentadiene	99.93	0.06	0.01	-
Isohexane	99.97	0.01	0.02	-
n-hexane	99.96	-	0.04	-
methylcyclopentane	99.95	0.02	0.03	-
benzene	98.89	1.00	0.11	-
toluene	98.80	0.81	0.39	-
m-xylene	97.91	0.86	1.20	0.03
styrene	96.65	1.85	1.46	0.04
dicyclopentadiene	98.55	0.63	0.80	0.02
naphthalene	42.27	20.56	36.33	0.81

** Distribution values determined using input data from the EPIWIN program experimental database

Test Substance:

The High Benzene Naphthas Category includes the following CAS numbers:

64741-99-7	Extracts, petroleum, light naphtha solvent
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-73-0	Naphtha, petroleum, hydrodesulfurized light
64742-83-2	Naphtha, petroleum, light steam-cracked
64742-91-2	Distillates, petroleum, steam-cracked
67891-79-6	Distillates, petroleum, heavy aromatic
67891-80-9	Distillates, petroleum, light aromatic
68410-97-9	Distillates, petroleum, light distillate hydrotreating process, low-boiling
68475-70-7	Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68526-77-2	Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum
68606-10-0	Gasoline, pyrolysis, debutanizer bottoms
68606-28-0	Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic
68921-67-5	Hydrocarbons, ethylene-manufacture-by-product distillation residues
68955-29-3	Distillates, petroleum, light thermal cracked, debutanized aromatic
68956-52-5	Hydrocarbons, C4-8
68956-70-7	Petroleum products, C5-12, reclaimed, wastewater treatment
69013-21-4	Fuel oil, pyrolysis
8030-30-6	Naphtha

	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The partitioning data represent a potential distribution range for substances in the 19 CAS numbers listed under Test Substance. Substances in the High Benzene Naphthas Category are calculated to partition primarily to air with a small percentage partitioning to water, soil, and sediment. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category. The input data used to run the EQC Level I model included estimated values calculated by the EPIWIN program based on chemical structure and measured data from the EPIWIN database. A comparison of the distribution data developed using either all calculated input values or measured values where data were available indicate a similar partitioning behavior and support the use of the dataset for chemicals without any measured data.
Reliability:	(2) Reliable with restrictions The input data used to run the EQC Level I model include calculated and experimental values available through the EPIWIN program. The data represent a potential environmental distribution range for substances with the 19 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E569

Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Transport-Distribution. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E562

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E562

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

Calculated and measured vapor pressure data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential vapor pressure range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific vapor pressure value. Actual vapor pressure ranges for substances in this category will vary dependent on their constituent composition.

Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the vapor pressure range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

Substance Constituent	Calculated VP (hPa @ 25°C)	Measured* VP (hPa @ 25°C)
Isoprene	7.35 E^2	7.33 E^2
n-pentane	6.84 E^2	6.85 E^2
1,3-cyclopentadiene	5.69 E^2	5.80 E^2
Isohexane	2.48 E^2	2.53 E^2
n-hexane	2.00 E^2	2.01 E^2
methylcyclopentane	1.77 E^2	1.84 E^2
benzene	1.16 E^2	1.26 E^2
toluene	31.60	37.86
m-xylene	8.83	11.05
styrene	6.73	8.53
dicyclopentadiene	2.20	3.05
naphthalene	0.05	0.11

* Experimental values from EPIWIN database.
The data represent a potential vapor pressure range for substances represented by the 19 CAS numbers under Test Substance.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E562

Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6

Robust Summary No.: OP E562

Conclusion:	The calculated vapor pressures for some representative constituents that are present in the category streams vary from 0.05 to 7.35 E^2 hPa @ 25°C. The measured vapor pressures of these same constituents vary from 0.11 to 7.33 E^2 hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Vapor pressure values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Vapor Pressure. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E564

HIGH BENZENE NAPHTHAS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6]
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". *Environ. Toxicol. Chem*. 15:100-106. 1995.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured water solubility data for representative constituents of the High Benzene Naphthas Category are listed below. The data identify a potential water solubility range for substances represented by the 19 CAS numbers under Test Substance. Substances in this category do not have a specific water solubility value. Actual water solubility ranges for substances in this category will vary dependent on their loading rate (i.e., weight of test material added to a volume of water). Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. The 12 chemicals selected to represent the water solubility range of this category are C5-C10 hydrocarbons that can be found in substances identified by the 19 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

CAS No.: 64741-99-7; 64742-49-0; 64742-73-0; 64742-83-2; 64742-91-2; 67891-79-6; 67891-80-9; 68410-97-9; 68475-70-7; 68476-45-9; 68526-77-2; 68606-10-0; 68606-28-0; 68921-67-5; 68955-29-3; 68956-52-5; 68956-70-7; 69013-21-4; 8030-30-6
Robust Summary No.: OP E564

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated WS (mg/L @ 25°C) / Measured WS* (mg/L @ 25°C) Isoprene 247.2 338.6 n-pentane 159.70 49.8 1,3-cyclopentadiene 470.6 na Isohexane 66.94 31.1 n-hexane 57.42 17.2 methylcyclopentane 83.95 49.4 benzene 2634.0 2000.0 toluene 832.7 573.1 m-xylene 258.4 207.2 styrene 386.7 343.7 dicyclopentadiene 51.9 na naphthalene 183.8 142.1 * Experimental values from EPIWIN database. na = not available The data represent a potential water solubility range for substances represented by the 19 CAS numbers under Test Substance.
Test Substance:	The High Benzene Naphthas Category includes the following CAS numbers: 64741-99-7 Extracts, petroleum, light naphtha solvent 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-73-0 Naphtha, petroleum, hydrodesulfurized light 64742-83-2 Naphtha, petroleum, light steam-cracked 64742-91-2 Distillates, petroleum, steam-cracked 67891-79-6 Distillates, petroleum, heavy aromatic 67891-80-9 Distillates, petroleum, light aromatic 68410-97-9 Distillates, petroleum, light distillate hydrotreating process, low-boiling 68475-70-7 Aromatic hydrocarbons, C6-8, naphtha-raffinate pyrolyzate-derived 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68526-77-2 Aromatic hydrocarbons, ethane cracking scrubber effluent and flare drum 68606-10-0 Gasoline, pyrolysis, debutanizer bottoms 68606-28-0 Hydrocarbons, C5 and C10-aliphatic and C6-8-aromatic 68921-67-5 Hydrocarbons, ethylene-manufacture-by-product distillation residues 68955-29-3 Distillates, petroleum, light thermal cracked, debutanized aromatic 68956-52-5 Hydrocarbons, C4-8 68956-70-7 Petroleum products, C5-12, reclaimed, wastewater treatment 69013-21-4 Fuel oil, pyrolysis 8030-30-6 Naphtha

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Test Substance: (cont'd)	High Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 19 CAS numbers are used to describe the ten process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry that contain significant levels of benzene, generally with a benzene content greater than 10% and averaging about 55%. More information on the High Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The High Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The calculated water solubility for some representative constituents that are present in the category streams vary from 51.9 to 2634.0 mg/L @ 25°C. The measured water solubility of these same constituents vary from 17.2 to 2000.0 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside of these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the 19 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the High Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Water solubility values were calculated by the WSKOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Water Solubility. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.